

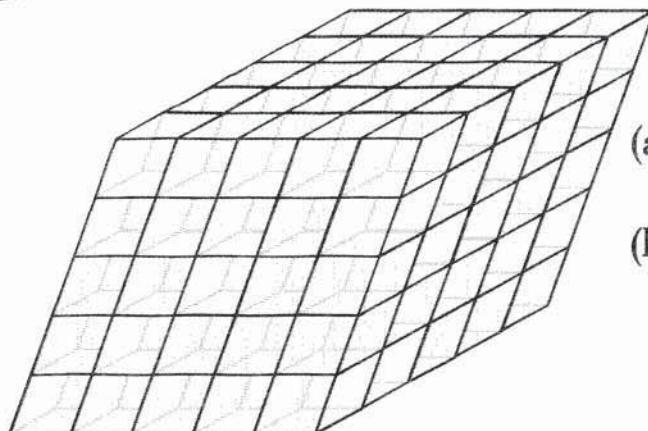
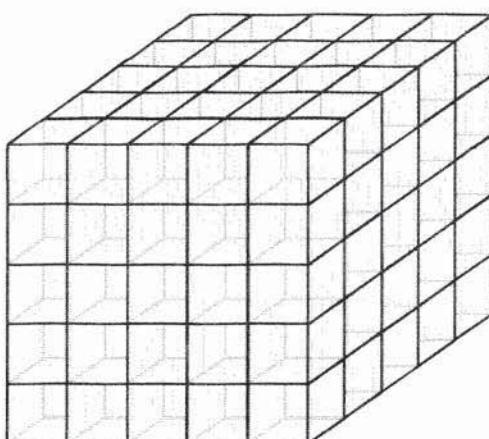
CHAPTER TWO

DEFORMATION OF MATTER

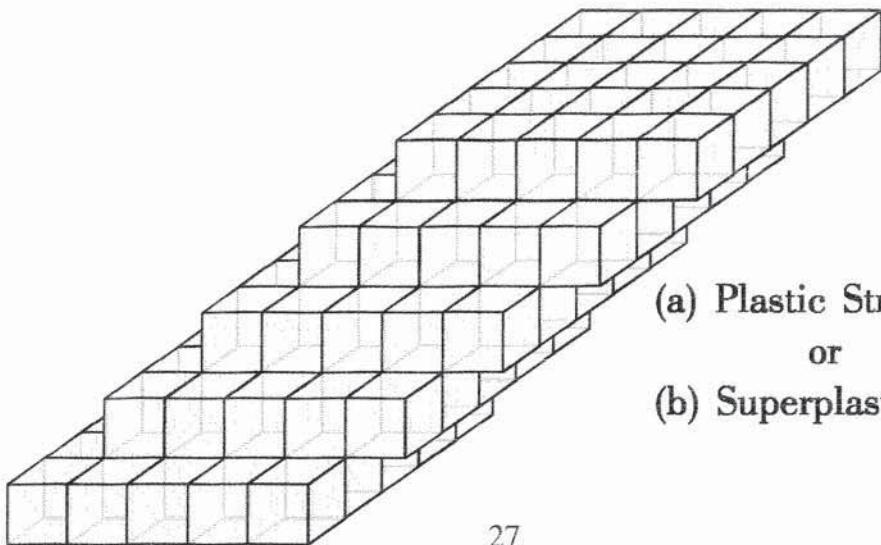
σ

Blocks Represent:

- (a) Unit Atomic Cells
or
- (b) Grains (Crystallites)



- (a) Elastic Strain
or
- (b) Creep



- (a) Plastic Strain
or
- (b) Superplastic Strain

Elastic deformations are reversible since matter is not redistributed but only displaced from equilibrium by a force. Thus, if the force is removed matter returns to its original, equilibrium position. "*The energy of an elastic deformation is nothing but energy put into the bonds between atom and atom by the deformation*" (Misner *et al.* 1973). Sufficiently large forces produce some type of *plastic deformation*: matter is redistributed by forces applied to material boundaries. It is an inherently *irreversible process*: if the forces are removed the material remains deformed; if they are reversed and moved over exactly the same distances which lead to the original deformation, it is highly unlikely that the initial condition is recovered. Plastic deformation permanently alters the microstructure of the material such that the original "path" no longer exists. It is also highly unlikely that reversed loads are applied precisely enough to properly engage the microstructural "agents" (*e.g.* dislocations) of deformation so that a reversed "path" is actually traversed by these "agents."

Atoms (10^{-8} cm) \rightarrow dislocations (10^{-4} cm) \rightarrow work-hardening (1 cm) (Misner *et al.* 1973).

Externally applied forces perform work per unit volume, W , on a body. The power input per unit volume to the body, P_{in} , produces both kinetic energy and stress energy; the latter is given by $P_s = \sigma \dot{\varepsilon}$, where σ is the stress and $\dot{\varepsilon}$ the strain rate (Reiner 1958). In isotropic materials the stress power is the sum of two independent terms: (1) an elastic term representing the volume change and (2) a plastic or distortional term that represents the body's shape change. At strain rates characteristic of superplastic flow the strain rate is so

small that the kinetic energy of the body can be neglected; thus, $P_{\text{in}} \approx P_o$ is a good approximation. The stress power complies with two thermodynamic laws embodied in the *Gibbs-Helmholtz equation*: $-\delta W = \delta G - \delta \varphi$, $\delta \varphi = 0$; here, δW is a "variation" in the work performed on a body, G is the free energy, and φ is the "bound energy."^[3] This equation expresses the condition that while at thermodynamic equilibrium $\delta \varphi = 0$, otherwise $\delta \varphi > 0$. For a body that obeys Hooke's law^[4] $\delta \varphi \equiv 0$. During Newtonian flow the elastic stress power is conserved and the distortional stress power is dissipated. In a general rheological process of real materials both functions G and φ are involved. For example, the flow stress of most superplastic materials is not linear in the strain rate; instead, $\sigma \propto \dot{\varepsilon}^m$, where $m \leq 1$ denotes the *strain rate sensitivity*. When $m < 1$, flow is non-Newtonian and the microstructure affects, and is also influenced by flow (*e.g.* deformation-enhanced grain growth). For a polycrystalline material the strain rate sensitivity is in general a function of the strain, strain rate, deformation temperature, grain size, grain size distribution, and other microstructural variables such as crystallographic texture that are not treated at all here.

[3]: See the next box, which indicates that the *virtual variation in bound energy*, $\delta \varphi$, is $\delta \varphi \equiv \delta E - T \delta S - \sum_{\alpha} \mu_{\alpha} \delta n^{\alpha} - \Gamma \delta A_v$. Here, E is the internal energy, T the temperature, S the entropy, μ_{α} the chemical potential of constituent α , and n^{α} the number of moles of α .

[4]: Meaning a *thermoelastic* material.

Thermodynamics Refresher

First law of thermodynamics: $dE = \Delta q + \Delta W + \sum_{\alpha} \mu_{\alpha} dn^{\alpha} + \Gamma dA_v$; here, E is the *internal energy* (e.g. per unit volume) of the system, q is the *heat supplied to the system*, W is the *work performed on the system*, Γ is the *surface tension*, A_v is the *grain boundary area per unit volume*; n^{α} denotes number of moles of α per unit volume, and the *chemical potential* of α is μ_{α} . *Second law of thermodynamics:* there is an *entropy function*, S , such that $dS = \Delta q/T$ for all *reversible processes* and $dS > \Delta q/T$ for all *irreversible processes*. The temperature, T , is an *integrating factor* since it converts the "inexact differential" Δq to the "exact differential" dS . Entropy and internal energy are *state functions*: $\oint dS = 0$ and $\oint dE = 0$. The work W is not generally a state function, $\oint dW \neq 0$, ΔW is "inexact," i.e. there is no thermodynamic function f such that $dW = \sum_{\alpha} (\partial f / \partial X^{\alpha}) dX^{\alpha}$, X^{α} representing thermodynamic variables, e.g. T , pressure (p), A_v , and n^{α} : e.g. $W(path, \sigma \Delta \varepsilon) = \int_{path} \sigma d\varepsilon$, ε denoting the strain and *path* the (unspecified) "parameterization" for the "object" $\sigma \Delta \varepsilon$. Variables are written as differentials (dX^{α}) to represent "infinitesimal increments." The *Gibbs free energy*, G , is, $G \equiv E + pV - TS = \sum_{\alpha} \mu_{\alpha} n^{\alpha}$, another state function; $dG = -SdT + Vdp + \sum_{\alpha} \mu_{\alpha} dn^{\alpha} + \Gamma dA_v$, where V is the volume of the material; $[dG]_{T,p} = \text{maximum work available from the system other than } -p\Delta V \text{ work}$ (Atkins 1978). The *equilibrium criteria* (Lupis 1983) is $(\delta G)_{T,p} = (\delta E - \delta W - T\delta S - \sum_{\alpha} \mu_{\alpha} \delta n^{\alpha} - \Gamma \delta A_v)_{T,p} \geq 0$: "at constant temperature and pressure the only possible variations which do not result in an irreversible process must increase the free energy of the system, i.e., at equilibrium the free energy is a minimum."

The tensile specimen is divided into *blocks of matter* that are comprised of *corpuscles* which are either atoms or grains, for deformation of a single crystal or polycrystalline material, respectively. For example, Nabarro (1967) emphasizes the primitive unit cell of a crystal lattice in his book on dislocation theory. *Differential geometry* is a tool for "counting up space" (Misner *et al.* 1973), and it is used for this purpose here.

Atoms are displaced slightly from equilibrium positions for elasticity and move from one equilibrium position to another for plasticity. The types of deformation of a polycrystalline material considered here are creep and superplasticity: creep results from small displacements of adjacent grains such that nearest neighbors remain nearest neighbors while superplasticity results from relative grain motions, *i.e.* neighbor switching. Grains stretch during creep and grain boundary area consequently increases, but during superplastic flow grains undergo mostly relative motions and, if there is no grain growth, the grain boundary area is *constant* (Ashby and Verrall 1973). Creep therefore corresponds (loosely) to crystal elasticity and superplasticity to crystal plasticity. This is the paradigm shift suggested by Morral and Ashby (1974) (although they did not consider creep). It is exploited here by using dislocation theory to discuss superplasticity; in particular the non-linear viscosity, or strain rate dependence of the strain rate sensitivity, and deformation-enhanced grain growth.

Grains (10 μm) \rightarrow clumps of grains (100 μm) \rightarrow viscosity (1 cm).

The viscosity observed results from how the microstructure changes with strain rate (*e.g.* grain growth) and how the motions of grain "clumps" changes with strain rate.

Having subdivided matter into appropriate corpuscles, *complexions*, or groups of corpuscles can be considered. Complexions can be defined such that some number of identical ones can be assembled to make a model for a tensile specimen. The tensile specimen is then "discretized," or "geometrized." For the case of corpuscles being grains and the tensile specimen a superplastic material, setting up the problem in this manner is also part of the problem, and one that has receive hardly, if any attention: What is the number of grains required of a complexion to fully model the behavior of the tensile specimen? This important question is not answered here, but the procedure, largely influenced by Rachinger (1952-53), should help: Grains stretch (creep), move (flow), and if there is grain growth, disappear from the microstructure, and if fracture is not considered, then these processes must occur such that the microstructure fills space without gaps.

The Model: To describe creep and superplasticity the polycrystalline microstructure is modelled as an "elasto-plastic froth." "Dual" to the froth is a lattice, constructed such that each point represents one cell. The froth has a surface tension (cohesion) and therefore resists stretching (creep). Energy in this froth is not instantly released when the stress is removed, in contrast to an atomic lattice; it is released slowly through the elimination of cells (grain growth). If the froth is stretched too much planes of cells roll over each other (superplasticity). This rolling occurs sequentially at the "irregular cells," or defects in the froth. These defects are cellular dislocations and disclinations. "Slip" occurs at these defects because they are associated with cells that are smaller than average. Defects exert "forces" on each other as well as neighboring cells, the latter causes coarsening (grain growth).

Modelling the Polycrystalline Microstructure

"Of course, idealization is a valid procedure in science, provided it is done consciously. But it is difficult to sustain a picture of many natural structures as imperfect realizations of some ordered ideal, from which they are distantly removed" (Weaire and Rivier 1984).

Polycrystalline materials, foams, and (biological) tissues are all examples of *random cellular arrays* (Weaire and Rivier 1984) that fill the space they occupy without gaps or overlaps. All these cell types have surface tension. Matzke (1946) studied cell shapes in foam and found that there were very many, none of which looked like Kelvin's tetrakaidecahedron, they were all irregular. Casual examination of the microstructure of a polycrystalline material suggests the same; see also Desch (1919). All of these structures are *disordered* (Weaire and Rivier 1984).

The typical two dimensional idealization of a polycrystalline microstructure is a honeycomb array; the "dual" to this cellular array is a lattice with *sixfold* symmetry. Sometimes an array of tetrakaidecahedron are used for, perhaps, a somewhat less idealistic representation (since it is three dimensional). If dislocations are introduced into the array of tetrakaidecahedron, then some cells have irregular shapes (Morral and Ashby 1974). A crude model for the grain size distribution of a polycrystalline material results.

Modelling the Polycrystalline Microstructure

(Continued)

"Some liquids display considerable short range order" and can therefore be modelled as "a solid densely packed with dislocations" (Nabarro 1967), suggestive of an amorphous state. The *amorphous state* has minimal symmetry (Rivier 1979). Long range order is totally absent in the amorphous state, but there are "remarkable" similarities between the amorphous and crystalline states of a substance (Venkataraman and Sahoo 1985). Atoms in metallic glasses are arranged in densely-packed spheres, while those in covalent glasses form *continuous random networks* (Venkataraman and Sahoo 1985). So, **modelling a polycrystalline microstructure as an amorphous substance, i.e. a cellular array densely packed with cellular dislocations, is a further advancement away from idealization.** This is the model of a polycrystalline material considered here. It is more idealistic than treating the microstructure as a random cellular array, but it offers mature descriptive methodology—dislocation theory.

See Fortes and Ferro (1985), Carnal and Mocellin (1981), and Kurtz and Carpay (1981) for discussion of polycrystalline microstructures; Weaire and Rivier (1984) and Rivier (1983,1985,1987) for descriptions of general, random cellular networks; and Venkataraman and Sahoo (1985,1986) and Rivier (1979,1987) for descriptions of defects in the amorphous state, and Chandrasekhar and Ranganath (1986) for defects in liquid crystals.

Misner *et al.* (1973) suggest the use of differential forms, or completely anti-symmetric, covariant tensors,^[5] for crystallography. In fact this has been done by many others to varying extents: see, for example, Bilby (1960), Kondo (1964), Nabarro (1967), Marcinkowski (1977,1979), Edelen (1979), Gairola (1979), Dzyaloshinskii and Volovick (1980), de Wit (1981), Kröner (1981,1990,1992), and Kröner and Lagoudas (1992). Venkataraman and Sahoo (1985,1986) provide a brief introduction for some of this material and discuss applications to describing defects in amorphous materials. Dereli and Vercin (1987) use the exterior calculus explicitly to describe defects in amorphous materials. Kröner (1990) makes extensive use of it for defects in crystalline materials. This approach is followed here; background material is provided to make it accessible. Much of the cited work actually adapts the continuum approach, but Kröner (1992) offers a rather complete crystallographic account, as does Marcinkowski (1977,1979).

Briefly, functions are "0-forms," covariant vectors are "1-forms," antisymmetric tensors with two "lower" indices are "2-forms," and antisymmetric tensors with three "lower" indices are "3-forms." The exterior derivative operator, \vec{d} , acts on a " p -form" and produces a " $(p + 1)$ -form:" so the exterior derivative of a function f is similar to its gradient $\vec{df} = \nabla f$; the exterior derivative of a covariant vector \mathbf{v} is similar to its curl, $\vec{d}\mathbf{v} = \nabla \times \mathbf{v}$; the exterior derivative of an antisymmetric tensor T with components $T_{ab} = -T_{ba}$ is similar to its divergence, $\vec{dT} = \nabla \cdot T$; and if a tensor T has antisymmetric components T_{abc} , then $\vec{dT} = \mathbf{0}$ identically ("3-forms" are "closed") in a "space" with three dimensions. I employ Misner *et al.*'s (1973) notation and definitions here, except that my \vec{d} equals their d .

[5]: *Tensors* are *invariant* functions for vectors and differential forms.

"Physical problems" are often translated into differential equations that when solved give the "solution" to the "problem." For example,

$$M(x,y,z)dx + N(x,y,z)dy + P(x,y,z)dz = 0 \quad \text{---} \quad \text{Eq. 1}$$

is a *linear, homogeneous, first-order differential equation*. The solution can therefore be obtained by integration, if the equation is in fact "integrable." This equation looks like a "covariant" vector, say \mathbf{v} , where $v_x \equiv M$, $v_y \equiv N$, $v_z \equiv P$: with $d\rho \equiv \mathbf{i}dx + \mathbf{j}dy + \mathbf{k}dz$, $\mathbf{v} \cdot d\rho = Mdx + Ndy + Pdz \equiv v_x dx + v_y dy + v_z dz$. The expression $\mathbf{v} \cdot d\rho = 0$ defines a plane with a normal vector \mathbf{v} ; $d\rho$ lies in the plane. The differential equation is "exact" in some "simply connected region" if $\nabla \times \mathbf{v} = \mathbf{0} \Rightarrow \partial M / \partial y = \partial N / \partial x$, $\partial M / \partial z = \partial P / \partial x$, $\partial N / \partial z = \partial P / \partial y$. The expression $\nabla \times \mathbf{v} = \mathbf{0}$ indicates that there is a function f such that $\mathbf{v} = \nabla f$ because $\nabla \times \nabla f = \mathbf{0}$ identically: the curl of a gradient always vanishes (a *vector identity*). So if the differential equation is "exact," then $df = Mdx + Ndy + Pdz = 0$, where $df \equiv (\partial f / \partial x)dx + (\partial f / \partial y)dy + (\partial f / \partial z)dz \equiv \nabla f \cdot d\rho \equiv \mathbf{v} \cdot d\rho$. Then the *solution* to the differential equation is $f(x,y,z) = \int df + \text{constant} = 0$.

The "exterior derivative" of a function f , \vec{df} , is a "rigorous" version of df (Misner *et al.* 1973): $\vec{df} \equiv (\partial f / \partial x)\vec{dx} + (\partial f / \partial y)\vec{dy} + (\partial f / \partial z)\vec{dz}$ is an example of a *1-form*. Another example of a 1-form is the *covariant vector*, or *Pfaffian* $\mathbf{v} \equiv M\vec{dx} + N\vec{dy} + P\vec{dz} \equiv v_x \vec{dx} + v_y \vec{dy} + v_z \vec{dz}$, which is generally neither "exact" or "integrable." Objects such as $\vec{dx}, \vec{dy}, \vec{dz}$ and $\vec{du}, \vec{dv}, \vec{dw}$ are *cotangent basis vectors*, they are equivalent to the usual differentials dx, dy, dz and du, dv, dw .

The *gradient* of f , ∇f is proportional to the *level surfaces* of f , i.e. $f = \text{constant}$ (Boas 1983). The magnitude of ∇f , $\|\nabla f\|$, $\|\nabla f\| \equiv \nabla f \cdot (\mathbf{i} + \mathbf{j} + \mathbf{k})$, gives the rate at which f increases in the direction normal to its level surfaces. The rate at which f increases in some general direction specified by a vector \mathbf{u} is $\mathbf{u} \cdot \nabla f = u^x(\partial f / \partial x) + u^y(\partial f / \partial y) + u^z(\partial f / \partial z)$, which is called the *directional derivative* (Morse and Feshbach 1953). The vector $\mathbf{u} = (u^x, u^y, u^z)$ gives a direction, and so it is a *contravariant vector*. Covariant vectors are associated with surfaces (Schouten 1989); ∇ turns f into the contravariant vector ∇f , the operator $\vec{\mathbf{d}}$ produces a covariant vector $\vec{\mathbf{d}}f$. The object $\vec{\mathbf{d}}f$ operates on a vector \mathbf{u} to produce the number $\vec{\mathbf{d}}f(\mathbf{u}) \equiv \mathbf{u} \cdot \nabla f = u^x(\partial f / \partial x) + u^y(\partial f / \partial y) + u^z(\partial f / \partial z)$. The object $\vec{\mathbf{d}}f$ is *integrable*: $\int \vec{\mathbf{d}}f \equiv \int_p^q \nabla f \cdot d\mathbf{l} = \int_p^q df = f(p) - f(q)$; $d\mathbf{l} \equiv \mathbf{i}dx + \mathbf{j}dy + \mathbf{k}dz$ is the "usual notation" for the differential distance giving part of the *path* from p to q .

Consider the *mapping* $x = f(u, v)$, $y = g(u, v)$ of a region A from the xy -plane into a region B of the uv -plane. Then the *surface integral* of some function $H(x, y) = H[f(u, v), g(u, v)]$ is

$$\iint_A H(x, y) dx dy = \iint_B H[f(u, v), g(u, v)] J(x, y; u, v) du dv,$$

where

$$J(x, y; u, v) \equiv \begin{vmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} \end{vmatrix} \equiv (\partial x / \partial u)(\partial y / \partial v) - (\partial x / \partial v)(\partial y / \partial u)$$

is the *Jacobian* of the transformation $x, y \rightarrow u, v$. Here, the regions A and B are equivalent, thus the integrands are *invariant*; they represent the same "2-form."

For the mapping $x = f(u,v,w)$, $y = g(u,v,w)$, $z = h(u,v,w)$ of a region A from the "space" xyz into a region B of the space uvw , the *volume integral* of $H(x,y,z) = H[f(u,v,w),g(u,v,w),h(u,v,w)]$ is

$$\iint_A H(x,y,z) dx dy dz = \iint_B H[f(u,v,w),g(u,v,w),h(u,v,w)] J(x,y,z;u,v,w) du dv dw,$$

where

$$J(x,y,z;u,v,w) \equiv \begin{vmatrix} \frac{\partial x}{\partial u} & \frac{\partial x}{\partial v} & \frac{\partial x}{\partial w} \\ \frac{\partial y}{\partial u} & \frac{\partial y}{\partial v} & \frac{\partial y}{\partial w} \\ \frac{\partial z}{\partial u} & \frac{\partial z}{\partial v} & \frac{\partial z}{\partial w} \end{vmatrix} \equiv \mathbf{e}_u \bullet \mathbf{e}_v \times \mathbf{e}_w$$

is the Jacobian of the transformation $x,y,z \rightarrow u,v,w$ and the integrands represent the same "3-form." Here,

$$\mathbf{e}_\alpha \equiv (\partial x / \partial u^\alpha) \mathbf{i} + (\partial y / \partial u^\alpha) \mathbf{j} + (\partial z / \partial u^\alpha) \mathbf{k}, \quad \alpha = u, v, w = u^\alpha,$$

are the *tangent basis vectors* for the u,v,w coordinates. The *inverse of J* , J^{-1} , is

$$[J(x,y,z;u,v,w)]^{-1} \equiv J(u,v,w;x,y,z) \equiv \begin{vmatrix} \frac{\partial u}{\partial x} & \frac{\partial u}{\partial y} & \frac{\partial u}{\partial z} \\ \frac{\partial v}{\partial x} & \frac{\partial v}{\partial y} & \frac{\partial v}{\partial z} \\ \frac{\partial w}{\partial x} & \frac{\partial w}{\partial y} & \frac{\partial w}{\partial z} \end{vmatrix} \equiv \nabla u \bullet \nabla v \times \nabla w.$$

The *differential line element*, $(ds)^2$, is the invariant

$$(ds)^2 = G_{xx}(dx)^2 + G_{yy}(dy)^2 + G_{zz}(dz)^2,$$

$$= G_{uu}(du)^2 + G_{vv}(dv)^2 + G_{ww}(dw)^2 + 2G_{uv}dudv + 2G_{uw}dudw + 2G_{vw}dvdw;$$

$G_{\alpha\alpha}$ ($\alpha = u, v, w$) and $G_{\alpha\beta}$ ($\alpha \neq \beta$) are components of the *metric tensor* for the u, v, w coordinate system, $G_{\alpha\beta} \equiv \mathbf{e}_\alpha \cdot \mathbf{e}_\beta$; and $G_{xx} = G_{yy} = G_{zz} = 1$ and $G_{xy} = G_{xz} = G_{yz} = 0$ are the same for the x, y, z coordinates, $G_{\alpha\beta} \equiv \mathbf{i}_\alpha \cdot \mathbf{i}_\beta = 1$ (0) if $\alpha = \beta$ ($\alpha \neq \beta$). Denoting determinants of the matrices obtained from components of the metric tensors by $|\mathbf{G}(u, v, w)|$ and $|\mathbf{G}(x, y, z)|$, then (Levi-Cevita 1977)

$$|\mathbf{G}(u, v, w)| = |\mathbf{G}(x, y, z)| |J(x, y, z; u, v, w)|^2.$$

The unit vectors $\mathbf{i}, \mathbf{j}, \mathbf{k}$ are equivalent to the *operators* $\partial/\partial x, \partial/\partial y, \partial/\partial z$ and, only because the x, y, z coordinates are *orthonormal* (i.e. $G_{\alpha\beta} = \delta_{\alpha\beta} \equiv$ Kronecker delta), they are also equivalent to $\vec{dx}, \vec{dy}, \vec{dz}$. Similarly for the u, v, w coordinates the tangent basis vectors are equivalent to $\mathbf{e}_\alpha \equiv \partial/\partial u^\alpha$ ($\alpha = u, v, w = u^\alpha$) (Misner *et al.* 1973). If $|\partial(\dots)/\partial x^\alpha|$ and $|\partial(\dots)/\partial u^\alpha|$ mean *consider the determinants as operators*

$$|\partial(\dots)/\partial x^\alpha| \equiv \begin{vmatrix} \partial(\dots)/\partial x & \partial(\dots)/\partial y & \partial(\dots)/\partial z \\ \partial(\dots)/\partial x & \partial(\dots)/\partial y & \partial(\dots)/\partial z \\ \partial(\dots)/\partial x & \partial(\dots)/\partial y & \partial(\dots)/\partial z \end{vmatrix} \equiv |\mathbf{i}_\alpha|$$

and,

$$|\partial(\dots)/\partial u^\alpha| \equiv \begin{vmatrix} \partial(\dots)/\partial u & \partial(\dots)/\partial v & \partial(\dots)/\partial w \\ \partial(\dots)/\partial u & \partial(\dots)/\partial v & \partial(\dots)/\partial w \\ \partial(\dots)/\partial u & \partial(\dots)/\partial v & \partial(\dots)/\partial w \end{vmatrix} \equiv |\mathbf{e}_\alpha|,$$

then (Levi-Cevita 1977)

$$|\partial(\dots)/\partial u^\alpha| = J(x^\alpha; u^\alpha) |\partial(\dots)/\partial x^\alpha|.$$

Here, the determinant $J(x^\alpha; u^\alpha)$ and "operator-determinant" $|\partial(\dots)/\partial x^\alpha|$ are multiplied like matrices. The relationships $|\mathbf{G}(u^\alpha)| = |\mathbf{G}(x^\alpha)| |J(x^\alpha; u^\alpha)|^2$ and $|\partial(\dots)/\partial u^\alpha| = J(x^\alpha; u^\alpha) |\partial(\dots)/\partial x^\alpha|$ imply that the contravariant version of the *Levi-Cevita tensor*, ϵ , is

$$\epsilon(\dots, \dots, \dots) \equiv |\mathbf{G}(u^\alpha)|^{-1/2} |\partial(\dots)/\partial u^\alpha| \equiv |\mathbf{G}(x^\alpha)|^{-1/2} |\partial(\dots)/\partial x^\alpha|.$$

It is a function for three 1-forms. The covariant version, discussed in the next sub-section, is a "3-form" obtained by writing the inverses to the right hand sides of this expression. It is a function for three vectors.

For the theory of lattice defects reviewed here, u, v, w coordinates represent crystallographic directions, or "lattice lines," and "solutions" to the "problem" give these coordinates as functions of x, y, z . It is "natural" to consider how functions change along the crystallographic directions: let \mathbf{e}_α denote tangent basis vectors for the crystallographic coordinates; the "covariant derivative operator," $\nabla_{\mathbf{e}_\alpha}$, is the tool to examine these changes. This operator is a "generalization" of the exterior derivative operator (Misner *et al.* 1973).

Direction of the Chapter

Section 1 introduces differential forms and provides some applications. For example, crystallography is treated with these tools: Pairs of planes from the family {100} are equivalent to the 1-forms which are the cotangent basis vectors for the crystallographic coordinate system based on conventional unit cells; directions from the family <100> are tangent basis vectors for this unit cell.^[6] The body-centered cubic crystal structure is "dual" to a regular stack of tetrakaidecahedrons; a lattice with *sixfold* symmetry is "dual" to a honeycomb array (Morral and Ashby 1974). Cellular arrays can therefore be treated idealistically as lattices. A review of the exterior calculus is provided here because an introductory treatment suitable to those interested in describing defects in solids is unavailable, even though it is somewhat in vogue. The review leads to a discussion of Pfaff's problem (Schouten and Kulk 1969), which Bilby (1960) and his coworkers recognized as applicable to dislocation theory. Some aspects of dislocation theory are introduced in this section using both exterior calculus/differential forms and vector analysis descriptions.

[6]: Standard crystallographic notation designates the directions [100],[010],[001] as the family <100> and the planes (100),(010),(001) as the family {100}. A *unit cell* is an elementary region of a crystal. It fills the space occupied by the crystal without overlaps or gaps when it is translated through some subset of the vectors of a Bravais lattice. A *Bravais lattice* consists of all points with position vectors ρ such that $\rho = I_1 \mathbf{A}_1 + I_2 \mathbf{A}_2 + I_3 \mathbf{A}_3$, where I_1, I_2, I_3 are integers and $\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3$ are not coplanar, *i.e.* $\mathbf{A}_1 \bullet \mathbf{A}_2 \times \mathbf{A}_3 \neq 0$. The vectors $\mathbf{A}_1, \mathbf{A}_2, \mathbf{A}_3$ are called *primitive lattice vectors*, and they generate the crystal structure. See Ashcroft and Mermin (1976).

Direction of the Chapter

(Continued)

Section 2 discusses elastic and dislocation deformations. In particular, a dislocation deformation from a single edge dislocation elastically deforms the surrounding lattice. The sum of these two deformations is compatible to first order (Nabarro 1967). A geometric description of compatibility is provided. Dislocations and disclinations are described. The Burgers vector and, torsion, curvature, and dislocation density tensors are defined, because these objects can all measure the Burgers vector. The Lie derivative is also discussed since it can be used to write the torsion and curvature tensors. The Lie derivative and torsion tensor measure the "anholonomic" ("non-conservative") nature of a vector field (Misner *et al.* 1973, Burke 1985): if the torsion tensor is non-zero then closed parallelograms can not be defined by "parallel transporting" two vectors along each other. If the curvature tensor, \mathbf{R} , is non-zero then a vector parallel transported along a closed path returns to its original position turned at an angle proportional to \mathbf{R} .

Section 3 is a presentation of "conventional" creep. A creep deformation stretches grains "compatibly;" it is "elastic-like" since no relative grain motions are presumed to take place. Cellular dislocations and disclinations affect the distribution of cell boundaries in the array; "compatibility" for these defects is discussed, after, for example, Rivier (1985).

Section 4 is about crystal plasticity from dislocation motion. The Peach-Koehler equation is derived. The applicability of Killing's equation to crystal plasticity is suggested. The Orowan equation is derived from the dislocation movement tensor. The tensile specimen and dislocation slip are "geometrized." And constitutive relationships are discussed.

Direction of the Chapter

(Continued)

Section 5 describes superplasticity with cellular dislocation motion, after Morral and Ashby (1974). The description is entirely analogous to that for crystal plasticity from the motion of lattice dislocations. The neighbor switching mechanisms for superplastic deformation from Lee (1970), Ashby and Verrall (1973), and Beeré (1976), are analyzed. Beeré's mechanism is found to be "slip-like" for a lattice with *sixfold* symmetry. Cellular dislocation glide is equivalent to "Rachinger grain boundary sliding," or neighbor switching, and models the translatory grain motion that is the most characteristic feature of superplastic deformation. The strain rate is proportional to the cellular dislocation density. After these topics are discussed, Sherwood and Hamilton's (1994) work is summarized: Morral and Ashby's hypothesis that a strain rate dependent cellular dislocation density leads to non-Newtonian behavior is examined with data obtained from Clark and Alden's single phase Sn-1% Bi alloy and a quasi-single phase 7475 Al alloy. Cellular dislocation climb models deformation-enhanced grain growth as well as translatory grain motion (Sato *et al.* 1990). The grain growth rate is also proportional to the cellular dislocation density (Morral and Ashby 1974). Two mechanisms for deformation-enhanced grain growth are presented: (1) thermally-activated and (2) stress-driven cellular dislocation climb. It is suggested that their grain growth kinetics are strain rate dependent, meaning that the first is most applicable for lower strain rates while only the latter is likely to be operable at higher strain rates. Grain growth kinetics are illustrated with Sn-1% Bi and 7475 Al data. Data for the 7475 Al alloy are given in the Appendix, which also discusses "non-ideal" grain growth.

§1. Subdivisions of Matter and Associated Introductory Notions

1.1. Vectors and Differential Forms in a Reference Frame

A *reference frame*, is a *coordinate system* established to make measurements with. I will only use the standard *Cartesian coordinates* $x,y,z \equiv \{x^a\} \equiv x^a$ for this; see Bilby *et al.* (1955) and Gairola (1979) for the general case. This coordinate system is *orthonormal*; *tangent basis vectors*, \mathbf{i}_a , are $\mathbf{i}_a \equiv \mathbf{i}, \mathbf{j}, \mathbf{k}$ and *cotangent basis vectors*, \mathbf{i}^a , are also $\mathbf{i}^a = \mathbf{i}, \mathbf{j}, \mathbf{k}$. The $\mathbf{i}, \mathbf{j}, \mathbf{k}$ have no units, whereas the units of x^a will either be Å or μm , for describing the positions of atoms or grains in tensile specimens made of a single crystal or polycrystal, respectively.

Contravariant components of a vector \mathbf{v} are v^a and *covariant components* are v_a ; $\mathbf{v} = v^a \mathbf{i}_a = v_a \mathbf{i}^a$ such that the components and basis vectors are summed over the indicial range $a = 1, 2, 3$ since they are "up" and "down," and "down" and "up," respectively (*summation convention*). Contravariant vectors can be represented by an arrow connecting two points while covariant vectors are represented by two planes, the distance between the planes being v_a (Schouten 1989).

The *metric* or *unit tensor*, \mathbf{G} , for the x^a coordinate system is $\mathbf{G} \equiv G_{ab} \mathbf{i}^a \otimes \mathbf{i}^b$, which is just $\mathbf{G} = \delta_{ab} \mathbf{i}^a \otimes \mathbf{i}^b = \mathbf{i} \otimes \mathbf{i} + \mathbf{j} \otimes \mathbf{j} + \mathbf{k} \otimes \mathbf{k}$, where $\delta_{ab} = 1$ if $a = b$ and $\delta_{ab} = 0$ if $a \neq b$ is the *Kronecker delta function*, \otimes is the *tensor product operator*, and since $\{x^a\}$ is orthonormal, $G_{ab} \equiv \mathbf{G}(\mathbf{i}_a, \mathbf{i}_b) = \mathbf{i}_a \bullet \mathbf{i}_b = \delta_{ab}$, ' \bullet ' denoting the *dot*, or *inner product operator*. The metric is used for two vectors, \mathbf{u} and \mathbf{v} , like $\mathbf{u} \bullet \mathbf{v} = u^a \mathbf{i}_a \bullet v^b \mathbf{i}_b \equiv u^a v^b G_{ab} \equiv u_b v^b = u v \cos \theta$, u and v denoting the magnitudes, or *norms* of \mathbf{u} and \mathbf{v} , *e.g.* $u^2 \equiv \mathbf{u} \bullet \mathbf{u} \equiv \|\mathbf{u}\|^2$, with θ being the angle between the vectors.

Tangent basis vectors are equivalent to the partial derivatives along the coordinate axes, $\mathbf{i}_a \equiv \partial/\partial x^a$, and the cotangent basis vectors are equivalent to the "differentials" \vec{dx}^a , as follows. The *directional derivative* of f along a vector \mathbf{v} is $\mathbf{v}[f] \equiv \partial_v f \equiv \mathbf{v} \cdot \vec{df} \equiv \langle \vec{df}, \mathbf{v} \rangle$ $\equiv \langle (\partial f/\partial x^a) \mathbf{i}^a, v^b \mathbf{i}_b \rangle \equiv (\partial f/\partial x^a) v^b \langle \mathbf{i}^a, \mathbf{i}_b \rangle \equiv (\partial f/\partial x^a) v^b \delta_a^b = (\partial f/\partial x^a) v^a$, where ' \vec{d} ' is the *exterior derivative operator*. Now drop the argument f in $\mathbf{v}[f] = (\partial f/\partial x^a) v^a$; $\mathbf{v}(\dots) \equiv \partial_v = v^a (\partial/\partial x^a)$, which suggests that $\mathbf{i}_a \equiv \partial/\partial x^a \equiv \vec{\partial}_a$, since $\mathbf{v} \equiv \sum_a v^a \mathbf{i}_a = v^x \mathbf{i}_x + v^y \mathbf{i}_y + v^z \mathbf{i}_z \equiv v^a \mathbf{i}_a$ is the usual definition of a vector (Misner *et al.* 1973). Similarly, $\vec{df} \equiv (\partial f/\partial x^a) \vec{dx}^a \equiv (\partial f/\partial x^a) \mathbf{i}^a$ looks just like the chain rule from calculus; the exterior derivative operator ' \vec{d} ' is a "rigorous" version of the usual differential operator 'd' (Misner *et al.* 1973); $\mathbf{i}^a \cdot \mathbf{i}_b \equiv \vec{dx}^a (\vec{\partial}_{x_b}) \equiv \langle \vec{dx}^a, \vec{\partial}_{x_b} \rangle \equiv \vec{\partial}_{x_b} (\vec{dx}^a) = \partial x^a / \partial x^b = \delta_a^b$ (Marsden and Hughes 1983). Note that the *bra-ket* notation, $\langle \dots, \dots \rangle$, is a "generalization" of the inner product; here $\langle \dots, \dots \rangle \equiv \dots \cdot \dots$, although other uses for $\langle \dots, \dots \rangle$ will arise. The first and second "slots" of $\langle \dots, \dots \rangle$ are for covariant and contravariant objects, respectively.

The cotangent basis vectors $\vec{dx}^a \equiv \mathbf{i}^a$ are *1-forms* that give the *level surfaces* $x^a = constant$. Any function f is a *0-form*, and then \vec{df} is the 1-form $\vec{df} = (\partial f/\partial x^a) \vec{dx}^a \equiv \partial_a f \vec{dx}^a = \partial_a f \mathbf{i}^a$, where $\partial_a f \equiv \partial f/\partial x^a$. The object \vec{df} is also an operator, $\vec{df} \equiv \vec{df}(\dots)$, taking a vector \mathbf{v} and producing the directional derivative, $\vec{df}(\mathbf{v}) \equiv \langle \vec{df}, \mathbf{v} \rangle \equiv \mathbf{v}[f]$, which is the number of f 's level surfaces pierced by \mathbf{v} ; and if $\mathbf{v} \rightarrow \mathbf{0}$, then this is just the difference in f , Δf , between the tip and tail of \mathbf{v} . It is also an integrand: $\int \vec{df} \equiv \int_p^q (\partial f/\partial x^a) \vec{dx}^a \equiv \int_p^q df = f(q) - f(p)$, where p and q are points. Similarly, the covariant form (or 1-form) of a vector \mathbf{v} , ${}^b \mathbf{v} = v_a \vec{dx}^a$, where ' b ' is the *flat operator*, is an object that can be integrated to provide the number of "standard lengths" (Burke 1985) of \mathbf{v} between the points p and q along some

path L , $\int_L^b \mathbf{v} = \int_L^b \frac{q}{p} \mathbf{v} \cdot d\mathbf{l}$, where $d\mathbf{l}$ is "standard" notation for the "differential distance" between points p and $p + \Delta p$; $\int_L^b \mathbf{v}$ is the number of surfaces of $v_a \vec{dx}^a$ "pierced" by L .

Covariant vectors $\overset{b}{\mathbf{v}} = v_a \vec{dx}^a$ are also called *Pfaffians* (Dodson and Poston 1979); they are generally not "gradients," *i.e.* a function f will probably not be available such that $v_a = \partial f / \partial x^a$. In this case the differential form is *inexact*, and Edelen (1985) refers to inexact 1-forms as Pfaffians. When a 1-form is a "gradient" its components can be expressed as $\partial f / \partial x^a$ and it is *exact* (Edelen (1985)). The *sharp operator*, '#' produces vectors out of 1-forms: *e.g.* $\# \vec{df} = (\partial f / \partial x^a) \mathbf{i}_a \equiv \nabla f$ is the *gradient* of f , where $\nabla \equiv \sum_a \mathbf{i}_a \partial / \partial x^a \equiv \mathbf{i} \partial / \partial x + \mathbf{j} \partial / \partial y + \mathbf{k} \partial / \partial z$.

Differential forms are completely *antisymmetric or alternating tensors* that represent stacks of "pieces" of space (Misner *et al.* 1973): 1-forms are stacks of "surfaces," *e.g.* \vec{dx} are "surfaces" perpendicular to the x -axis which give the number of y - z planes per unit length along the x -axis; 2-forms are stacks of "tubes," *e.g.*

$$\vec{dx} \wedge \vec{dy} = \begin{vmatrix} \vec{dx}(\dots) & \vec{dx}(\dots) \\ \vec{dy}(\dots) & \vec{dy}(\dots) \end{vmatrix}$$

are tubes "pointing" along the z -axis, which represent the number of "squares" $\vec{dx} \wedge \vec{dy}$ per unit area; and 3-forms, *e.g.* $\vec{dx} \wedge \vec{dy} \wedge \vec{dz}$, are "cubes" which give the number of points per unit volume (Misner *et al.* 1973, Burke 1985). Here, the vertical bars for $\vec{dx} \wedge \vec{dy}$ denote determinant of the matrix; the notation $\vec{dx}^a(\dots)$ means that this determinant is an operator without arguments, and is therefore a function for two vectors. Differential forms are

integrands: consider the surface integral $\iint Pdydz + Qdzdx + Rdxdy$, the integrand $Pdydz + Qdzdx + Rdxdy$ is equivalent to the 2-form $P\vec{dy} \wedge \vec{dz} + Q\vec{dz} \wedge \vec{dx} + R\vec{dx} \wedge \vec{dy}$, the obvious omission of terms such as $dxdx$ indicates skew symmetry (Flanders 1989).

The exterior derivative operator acts only on differential forms and functions. It has a "generalization," discussed in this Chapter's Appendix, which acts on vectors too.

The *wedge* or *exterior product*, \wedge , produces *skew symmetric (antisymmetric)* tensors from vectors:

$$\mathbf{u} \wedge \mathbf{v} \equiv \mathbf{u} \otimes \mathbf{v} - \mathbf{v} \otimes \mathbf{u};$$

$\mathbf{u} \wedge \mathbf{v}$ is a piece of a two dimensional, *oriented surface*, a *bivector*. Equivalently, for 1-forms (covariant vectors) ${}^b\mathbf{u} \wedge {}^b\mathbf{v} \equiv {}^b\mathbf{u} \otimes {}^b\mathbf{v} - {}^b\mathbf{v} \otimes {}^b\mathbf{u}$, where ${}^b\mathbf{u} \wedge {}^b\mathbf{v}$ is a 2-form (stack of "tubes").

Here,

$$\begin{aligned} {}^b\mathbf{u} \wedge {}^b\mathbf{v} &\equiv \sum_a u_a \vec{dx}^a \wedge \sum_b v_b \vec{dx}^b \equiv u_a \vec{dx}^a \wedge v_b \vec{dx}^b \\ &\equiv \sum_{a,b} u_a v_b \vec{dx}^a \wedge \vec{dx}^b \equiv u_a v_b \vec{dx}^a \wedge \vec{dx}^b, \\ &\equiv \sum_{a < b} (u_a v_b - u_b v_a) \vec{dx}^a \wedge \vec{dx}^b, \\ &\equiv \frac{1}{2} \sum_{a,b} (u_a v_b - u_b v_a) \vec{dx}^a \wedge \vec{dx}^b \equiv \frac{1}{2}(u_a v_b - u_b v_a) \vec{dx}^a \wedge \vec{dx}^b, \\ &= (u_y v_z - u_z v_y) \vec{dy} \wedge \vec{dz} + (u_z v_x - u_x v_z) \vec{dz} \wedge \vec{dx} + (u_x v_y - u_y v_x) \vec{dx} \wedge \vec{dy}. \end{aligned}$$

These formulas work for $\mathbf{u} \wedge \mathbf{v}$ too with the substitution of $\mathbf{i}_a \wedge \mathbf{i}_b$ for $\vec{dx}^a \wedge \vec{dx}^b \equiv \mathbf{i}^a \wedge \mathbf{i}^b$.

The wedge product is similar to the *vector or cross product*^[7] given by (Malvern 1969),

[7]: For example, a rigid body remains at rest if the sum of all 'n' forces \mathbf{F}^n on it

$$\begin{aligned}\mathbf{u} \times \mathbf{v} &\equiv \sum_{a,b} e_{abc} \mathbf{i}^a u^b v^c \equiv e_{abc} \mathbf{i}^a u^b v^c \equiv \frac{1}{2} e_{abc} \mathbf{i}^a (u^b v^c - u^c v^b), \\ &= (u^y v^z - u^z v^y) \mathbf{i}^x + (u^z v^x - u^x v^z) \mathbf{i}^y + (u^x v^y - u^y v^x) \mathbf{i}^z,\end{aligned}$$

$$= \begin{vmatrix} \mathbf{i} & \mathbf{j} & \mathbf{k} \\ u^x & u^y & u^z \\ v^x & v^y & v^z \end{vmatrix}.$$

Here, e_{abc} denote covariant components of the *permutation tensor*: $e_{abc} = 1$ for even permutations of a,b,c , $e_{abc} = -1$ for odd permutations, and $e_{abc} = 0$ if any two of the indices a,b,c are equal. If the vectors \mathbf{u} and \mathbf{v} have a common origin then they span a parallelogram, and the magnitude of the vector $\mathbf{w} \equiv \mathbf{u} \times \mathbf{v}$ is equal to the area of the parallelogram, and similarly for the bivector $\mathbf{u} \wedge \mathbf{v} \equiv \frac{1}{2}(u^a v^b - u^b v^a) \vec{\partial}_a \wedge \vec{\partial}_b$ (Misner *et al.* 1973). Finally, the *tensor product* is a function, $\mathbf{u} \otimes \mathbf{v} = \mathbf{u} \otimes \mathbf{v}(\dots, \dots)$, for two 1-forms, say ω and θ :

$$\mathbf{u} \otimes \mathbf{v}(\omega, \theta) \equiv \langle \omega, \mathbf{u} \rangle \langle \theta, \mathbf{v} \rangle \equiv (\omega \bullet \mathbf{u})(\theta \bullet \mathbf{v}) \equiv (\omega_a u^a)(\theta_b v^b).$$

Its antisymmetric nature aside, $\mathbf{u} \wedge \mathbf{v} = -(\mathbf{v} \wedge \mathbf{u})$, "familiar" rules of addition and multiplication hold for the wedge product:

$$\begin{aligned}(a\mathbf{u} + b\mathbf{v}) \wedge c\mathbf{w} &= ac(\mathbf{u} \wedge \mathbf{w}) + bc(\mathbf{v} \wedge \mathbf{w}), \\ (\mathbf{u} \wedge \mathbf{v}) \wedge \mathbf{w} &= \mathbf{u} \wedge (\mathbf{v} \wedge \mathbf{w}).\end{aligned}$$

If α is a p -form and β is a q -form, then

vanishes, $\sum_n F^n = \mathbf{0}$, and if the sum of the moments about some point ρ vanishes, $\sum_n (\rho^n - \rho) \wedge F^n = \mathbf{0}$ (Misner *et al.* 1973).

$$\alpha \wedge \beta = (-1)^{pq} \beta \wedge \alpha,$$

so long as $p + q \leq 3$, where $n = 3$ is the dimension of the "space;" if $p + q > 3$, then $\alpha \wedge \beta = 0$ because there would be terms such as $\vec{d}x \wedge \vec{d}x$ in the expression, and \wedge is antisymmetric so it would vanish (Flanders 1989). For example, the exterior product of a 1-form $\alpha = A\vec{d}x + B\vec{d}y + C\vec{d}z$ and a 2-form $\beta = P\vec{d}y \wedge \vec{d}z + Q\vec{d}z \wedge \vec{d}x + R\vec{d}x \wedge \vec{d}y$ gives the 3-form $\alpha \wedge \beta = (AP + BQ + CR)\vec{d}x \wedge \vec{d}y \wedge \vec{d}z$, which is equivalent to the dot product of α and β . Thus, the wedge product generalizes operators from vector analysis.

The 3-form $\vec{d}x \wedge \vec{d}y \wedge \vec{d}z$ is the *Levi-Cevita tensor*, which is the "dual" of unity, $*1$, $*1 = \epsilon$ (Misner *et al.* 1973), or *volume 3-form* (Burke 1985), since it gives the number of unit "cubes" per volume:

$$\epsilon \equiv \vec{d}x \wedge \vec{d}y \wedge \vec{d}z \equiv \sum_{a,b,c} e_{abc} \vec{d}x^a \otimes \vec{d}x^b \otimes \vec{d}x^c,$$

$$\equiv \begin{vmatrix} \vec{d}x(\dots) & \vec{d}x(\dots) & \vec{d}x(\dots) \\ \vec{d}y(\dots) & \vec{d}y(\dots) & \vec{d}y(\dots) \\ \vec{d}z(\dots) & \vec{d}z(\dots) & \vec{d}z(\dots) \end{vmatrix},$$

$$\equiv \vec{d}x \otimes \vec{d}y \otimes \vec{d}z + \vec{d}y \otimes \vec{d}z \otimes \vec{d}x + \vec{d}z \otimes \vec{d}x \otimes \vec{d}y \\ - \vec{d}x \otimes \vec{d}z \otimes \vec{d}y - \vec{d}y \otimes \vec{d}x \otimes \vec{d}z - \vec{d}z \otimes \vec{d}y \otimes \vec{d}x.$$

The notation $\vec{d}x^a(\dots)$ again means that this determinant ϵ is an operator without arguments in the slots (...); it is therefore a function for three vectors, $\epsilon = \epsilon(\dots, \dots, \dots)$. Since the $\mathbf{i}_a, \mathbf{i}^a = \mathbf{i}, \mathbf{j}, \mathbf{k}$ are orthonormal, the components of ϵ , ϵ_{abc} and ϵ^{abc} , are just the components of the permutation tensor, $\epsilon_{abc} = e_{abc}$ and $\epsilon^{abc} = e^{abc}$. This is not the case, however, for other, more "general" coordinate systems. Installing the basis vectors $\mathbf{i}_a \equiv \vec{d}_a$ into ϵ evaluates the determinant:

$$\epsilon(\vec{d}_x, \vec{d}_y, \vec{d}_z) \equiv \vec{d}x(\vec{d}_x)\vec{d}y(\vec{d}_y)\vec{d}z(\vec{d}_z) + 0 + 0 - 0 - 0 - 0 \equiv \mathbf{i} \cdot \mathbf{j} \times \mathbf{k} = 1.$$

The permutation tensor obeys the following relationships:

$$e^{abc} e_{ade} = \delta_d^b \delta_e^c - \delta_e^b \delta_d^c \text{ and } e^{abc} e_{abd} = 2\delta_d^c.$$

The *norm* of a p -form $\alpha \equiv \alpha_{|a_1 \dots a_p} \vec{d}x^{a_1} \dots \vec{d}x^{a_p} \equiv (1/p!) \alpha_{|a_1 \dots a_p} \vec{d}x^{a_1} \dots \vec{d}x^{a_p}$ gives the square of its magnitude,

$$\|\alpha\| \equiv \alpha \cdot \alpha \equiv \alpha_{|a_1 \dots a_p} \alpha^{a_1 \dots a_p} \equiv \alpha^2,$$

vertical bars denoting summation over the restricted range $a_1 < \dots < a_p$ (Misner *et al.* 1973). The *dual* of this p -form is the $(3 - p)$ -form ${}^*\alpha$:

$$\alpha \equiv \alpha_{|a_1 \dots a_p} \vec{d}x^{a_1} \dots \vec{d}x^{a_p} \Rightarrow {}^*\alpha \equiv \alpha^{[a_1 \dots a_p]} \epsilon_{a_1 \dots a_p \dots b_1 \dots b_{3-p}} \vec{d}x^{b_1} \dots \vec{d}x^{b_{3-p}},$$

with components

$$(*\alpha)_{b_1 \dots b_{3-p}} \equiv \alpha^{a_1 \dots a_p} \epsilon_{a_1 \dots a_p \dots b_1 \dots b_{3-p}} \equiv \frac{1}{p!} \alpha^{a_1 \dots a_p} \epsilon_{a_1 \dots a_p \dots b_1 \dots b_{3-p}}.$$

Meaning of the Dual *: The object $\int \alpha$ is the integral of the tangential component of α over a p -dimensional "surface" whereas the object $\int * \alpha$ is the integral of the normal component of α over a $(3 - p)$ -dimensional "surface" (Misner and Wheeler 1957).

A 1-form, $\alpha = \alpha_a \vec{dx}^a$, is a function to produce a number out of a (contravariant) vector, $\mathbf{u} = u^b \vec{\partial}_b$: $\langle \alpha, \mathbf{u} \rangle = \alpha_a u^b \langle \vec{dx}^a, \vec{\partial}_b \rangle = \alpha_a u^b \delta_a^b = \alpha_a u^a = \text{number of surfaces of } \alpha \text{ pierced by } \mathbf{u}$ (Misner *et al.* 1973). A 2-form

$$\mathbf{B} \equiv \beta_{[ab]} \vec{dx}^a \wedge \vec{dx}^b \equiv \frac{1}{2} \beta_{ab} \vec{dx}^a \wedge \vec{dx}^b, \beta_{ab} = -\beta_{ba},$$

vertical bars again denoting summation over the restricted range $a < b$, is a function to produce a number out of an *oriented surface*, $\mathbf{u} \wedge \mathbf{v}$, formed by the two vectors \mathbf{u} and \mathbf{v} (Misner *et al.* 1973): The number of tubes of \mathbf{B} cut through by surface $\mathbf{S} = \mathbf{u} \wedge \mathbf{v}$ is

$$\mathbf{B}(\mathbf{u}, \mathbf{v}) \equiv \langle \mathbf{B}, \mathbf{u} \wedge \mathbf{v} \rangle \equiv \langle \beta_{[ab]} \vec{dx}^a \wedge \vec{dx}^b, u^c \vec{\partial}_c \wedge v^d \vec{\partial}_d \rangle,$$

$$\equiv \beta_{[ab]} \begin{vmatrix} \langle \vec{dx}^a, \mathbf{u} \rangle & \langle \vec{dx}^a, \mathbf{v} \rangle \\ \langle \vec{dx}^b, \mathbf{u} \rangle & \langle \vec{dx}^b, \mathbf{v} \rangle \end{vmatrix}, \quad (\text{Flanders 1989})$$

$$\equiv \beta_{[ab]} u^c v^d \langle \vec{dx}^a \wedge \vec{dx}^b, \vec{\partial}_c \wedge \vec{\partial}_d \rangle,$$

$$= \beta_{[ab]} u^c v^d \delta_{cd}^{ab} = \beta_{[ab]} u^a v^b.$$

Here, $\delta_{cd}^{ab} \equiv \delta_c^a \delta_d^b - \delta_d^a \delta_c^b$ is a "permutation tensor": $\delta_{cd}^{ab} = 1$ if ab is an even permutation of cd, $\delta_{cd}^{ab} = -1$ if ab is an odd permutation of cd, and $\delta_{cd}^{ab} = 0$ otherwise. If \mathbf{S} is a large surface then $\int_S \mathbf{B}$ is the total number of "tubes" of \mathbf{B} cut by \mathbf{S} . A 3-form,

$$\gamma = \gamma_{abc} \vec{dx}^a \wedge \vec{dx}^b \wedge \vec{dx}^c = \frac{1}{3!} \gamma_{abc} \vec{dx}^a \wedge \vec{dx}^b \wedge \vec{dx}^c,$$

is a function such that if the vectors $\mathbf{u}, \mathbf{v}, \mathbf{w}$ form an *oriented volume* $\mathbf{u} \wedge \mathbf{v} \wedge \mathbf{w}$, then

$\langle \gamma, \mathbf{u} \wedge \mathbf{v} \wedge \mathbf{w} \rangle = \text{number of cells of } \gamma \text{ in volume } \mathbf{u} \wedge \mathbf{v} \wedge \mathbf{w}$:

$$\begin{aligned} \gamma(\mathbf{u}, \mathbf{v}, \mathbf{w}) &\equiv \langle \gamma, \mathbf{u} \wedge \mathbf{v} \wedge \mathbf{w} \rangle \equiv \gamma_{abc} u^d v^e w^f \langle \vec{dx}^a \wedge \vec{dx}^b \wedge \vec{dx}^c, \vec{d}_d \wedge \vec{d}_e \wedge \vec{d}_f \rangle, \\ &\equiv \gamma_{abc} u^d v^e w^f \delta_{def}^{abc}, \\ &= \gamma_{abc} u^a v^b w^c. \end{aligned}$$

Here, $\mathbf{u} \wedge \mathbf{v} \wedge \mathbf{w}$ is a *trivector*:

$$\mathbf{u} \wedge \mathbf{v} \wedge \mathbf{w} \equiv V^{xyz} \mathbf{i} \wedge \mathbf{j} \wedge \mathbf{k} \equiv \frac{1}{3!} \begin{vmatrix} u^x & u^y & u^z \\ v^x & v^y & v^z \\ w^x & w^y & w^z \end{vmatrix} \mathbf{i} \wedge \mathbf{j} \wedge \mathbf{k}.$$

The object $\mathbf{u} \wedge \mathbf{v} \wedge \mathbf{w}$ is a *simple trivector* because it is just a determinant of three vectors (Schouten 1989):

$$\begin{aligned} V^{xyz} &\equiv u^x(v^y w^z - w^y v^z) + u^y(v^z w^x - w^z v^x) + u^z(v^x w^y - w^x v^y) \equiv 3! u^x v^y w^z, \\ &\approx \mathbf{u} \bullet \mathbf{v} \times \mathbf{w}; \end{aligned}$$

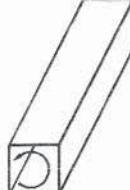
the permutation symbol, $[]$, on three indices meaning

$$u^{[m} v^n w^{p]} \equiv \frac{1}{3!}(u^m v^n w^p + u^n v^p w^m + u^p v^m w^n - u^m v^p w^n - u^n v^m w^p - u^p v^n w^m).$$

Clearly, all three of these differential forms, α , β , and γ , are useful tools for doing crystallography: counting planes of atoms, rows ("tubes") of atoms, and atoms (unit cells), respectively.^[8] And similarly for counting "sheets" of grains, "tubes" of grains, and grains. These objects, and others, are summarized in the following table. For this table, $e_\alpha \equiv \vec{\partial}_\alpha$ $\equiv \partial/\partial\chi^\alpha$ and $e^\alpha \equiv \vec{d}\chi^\alpha$ are tangent and cotangent basis vectors for some "general" coordinate system $\{\chi^\alpha\}$ and they are consequently not expected to be orthonormal. Of course, these definitions are applicable in any coordinate system, orthogonal or not.

[8]: For example, a dislocation core is a row of incorrectly bonded atoms, and one might therefore expect these line defects to be characterized by a 2-form.

TABULATION OF GEOMETRIC OBJECTS (Schouten 1954)[†]

Object	Name	Notation	Second Notation‡	Sense
\mathbb{R}	Scalar (0-form)	s	$*s \equiv se^1 \wedge e^2 \wedge e^3$ $\#(*s) \equiv se_1 \wedge e_2 \wedge e_3$	\pm sign
	Vector	$v \equiv v^\alpha e_\alpha \equiv v^\alpha \vec{d}_\alpha$	$\tilde{v} \equiv \epsilon_{\alpha\beta\gamma} v^\alpha e^\beta \wedge e^\gamma$	inner
	1-Form	$b_v \equiv v_\alpha e^\alpha \equiv v_\alpha \vec{d}\chi^\alpha$	$\tilde{b}_v \equiv \epsilon^{\alpha\beta\gamma} v_\alpha e_\beta \wedge e_\gamma$	outer
	Bivector	$\bar{A} \equiv u \wedge v \equiv A^{\alpha\beta} e_\alpha \wedge e_\beta$ $A^{\alpha\beta} \equiv 1/2(u^\alpha v^\beta - u^\beta v^\alpha)$	$\tilde{A} \equiv \epsilon_{\alpha\beta\gamma} A^{\alpha\beta} e^\gamma$ $\tilde{A}_\gamma \equiv \epsilon_{\alpha\beta\gamma} A^{\alpha\beta}$	inner
	2-Form	$B \equiv 1/2\beta_{\alpha\beta} e^\alpha \wedge e^\beta$ $\beta_{\alpha\beta} = -\beta_{\beta\alpha}$	$\tilde{B} \equiv \epsilon^{\alpha\beta\gamma} \beta_{\alpha\beta} e_\gamma$ $\tilde{\beta}^\gamma \equiv \epsilon^{\alpha\beta\gamma} \beta_{\alpha\beta}$	outer
	Trivector	$u \wedge v \wedge w$	$u^{[\alpha} v^\beta w^{\gamma]}$	screw
	3-Form	$\gamma \equiv 1/3\gamma_{\alpha\beta\gamma} e^\alpha \wedge e^\beta \wedge e^\gamma$	$\gamma_{[\alpha\beta\gamma]}$	

[†]See Misner *et al.* (1973) as well. See Burke (1985) and Schouten (1989) for other

objects.

[‡]The "second notation" is rarely used here. The symbol \sim will not always mean that I am using the second notation for an object; I will say so when this is the case.

Exterior differentiation obeys the rules (Misner *et al.* 1973)

$$\vec{d}(\alpha + \beta) \equiv \vec{d}\alpha + \vec{d}\beta$$

and, for α a p -form and β any form,

$$\vec{d}(\alpha \wedge \beta) \equiv \vec{d}\alpha \wedge \beta + \alpha \wedge (-1)^p \vec{d}\beta.$$

For example, the exterior derivative of a 1-form α produces the 2-form which is the *rotation* of α , $\text{rot } \alpha$,

$$\alpha = \alpha_a \vec{d}x^a \Rightarrow \vec{d}\alpha \equiv (\partial\alpha_a/\partial x^b) \vec{d}x^b \wedge \vec{d}x^a = \frac{1}{2}(\partial\alpha_a/\partial x^b - \partial\alpha_b/\partial x^a) \vec{d}x^b \wedge \vec{d}x^a;$$

the fact that $\vec{d}(\vec{d}x^a) = 0$ was used here. The rotation operation is analogous to the *curl* operation:

$$\text{curl } {}^b v \equiv \nabla \times {}^b v \equiv \epsilon^{abc} i_a \partial v_c / \partial x^b \equiv e^{abc} i_a \partial_b v_c \equiv \begin{vmatrix} i & j & k \\ \partial/\partial x & \partial/\partial y & \partial/\partial z \\ v_x & v_y & v_z \end{vmatrix},$$

where $\partial_b \equiv \partial/\partial x^b$; but $\epsilon^{abc} = e^{abc}$ only for the x^a coordinates. Exterior differentiation of a 2-form β produces a 3-form:

$$\beta \equiv \beta_{[ab]} \vec{d}x^a \wedge \vec{d}x^b \Rightarrow \vec{d}\beta \equiv \vec{d}\beta_{[ab]} \wedge \vec{d}x^a \wedge \vec{d}x^b = (\partial\beta_{[ab]}/\partial x^c) \vec{d}x^c \wedge \vec{d}x^a \wedge \vec{d}x^b.$$

This is similar to the divergence operation: the "second notation" for the 2-form \mathbf{B} is $\tilde{\mathbf{B}} \equiv \epsilon^{abc} \beta_{ab} \mathbf{i}_c$ and the *divergence* of $\tilde{\mathbf{B}}$ is

$$\operatorname{div} \tilde{\mathbf{B}} \equiv \nabla \cdot \tilde{\mathbf{B}} \equiv \partial_c \tilde{\beta}^c \equiv \frac{1}{2} \epsilon^{cab} \partial_{[c} \beta_{ab]},$$

where $\tilde{\beta}^c \equiv \epsilon^{abc} \beta_{ab}$ are the components of $\tilde{\mathbf{B}}$ (Schouten 1954).^[9] Exterior differentiation of a 3-form γ vanishes identically in a three dimensional space, $\vec{d}\gamma = 0$, since there are no 4-forms. The 3-form is therefore *closed* (Edelen 1985).

Finally, if ω is a p -form and \mathbf{v} is a vector, then the *interior product* is the $(p - 1)$ -form given by

$$\mathbf{v} \lrcorner \omega \equiv \frac{1}{(1-p)} v^b \omega_{ba_2 \dots a_p} \vec{d}x^{a_2} \dots \vec{d}x^{a_p},$$

where \lrcorner is the *interior product operator* (Marsden and Hughes 1983); rather little use will be made of it here.

[9]: Objects which have no divergence have no source; their "tubes" have no beginning and no end; so they are either closed, or extend from $-\infty$ to $+\infty$.

1.2. The Poincaré Lemma

I'll just state the lemma for reference, then motivate and discuss it in detail as if it had not been introduced:

Poincaré Lemma—If there is a "region of space," say \mathbf{U} , which can be shrunk to a point in a "smooth" way, then if $\vec{\mathbf{d}}\mathbf{B} = \mathbf{0}$ on \mathbf{U} , there exists a differential form, say $\boldsymbol{\alpha}$, such that $\mathbf{B} = \vec{\mathbf{d}}\boldsymbol{\alpha}$ (Edelen 1985). Equivalently: "Every closed form on \mathbf{U} is exact" (Edelen 1977).

Suppose that $\boldsymbol{\alpha} = \alpha_a \vec{\mathbf{d}}x^a$ where $\alpha_a = \partial f / \partial x^a \equiv \partial_a f$, i.e. that $\boldsymbol{\alpha} = \vec{\mathbf{d}}f$. Then

$$\begin{aligned}\boldsymbol{\alpha} &= \alpha_a \vec{\mathbf{d}}x^a, \quad \alpha_a \equiv \partial_a f \Rightarrow \vec{\mathbf{d}}\boldsymbol{\alpha} = \frac{1}{2}(\partial_b \alpha_a - \partial_a \alpha_b) \vec{\mathbf{d}}x^b \wedge \vec{\mathbf{d}}x^a, \\ &= \frac{1}{2}(\partial_b \partial_a f - \partial_a \partial_b f) \vec{\mathbf{d}}x^b \wedge \vec{\mathbf{d}}x^a, \\ &= \vec{\mathbf{d}}\vec{\mathbf{d}}f \equiv \vec{\mathbf{d}}^2 f = \mathbf{0}.\end{aligned}$$

The result $\vec{\mathbf{d}}^2 f = \frac{1}{2}(\partial^2 f / \partial x^b \partial x^a - \partial^2 f / \partial x^a \partial x^b) \vec{\mathbf{d}}x^b \wedge \vec{\mathbf{d}}x^a = \mathbf{0} \Rightarrow \partial^2 f / \partial x^b \partial x^a - \partial^2 f / \partial x^a \partial x^b = 0$ gives the *equality of mixed second partial derivatives*, which is the *Poincaré Lemma*, the source of most "*integrability conditions*" (Flanders 1989). It is equivalent to the "standard" result $\nabla \times {}^b \nabla f = \mathbf{0}$ from vector analysis; gradients are curl-free.

Suppose that the 2-form $\mathbf{B} \equiv \beta_{ab} \vec{\mathbf{d}}x^a \wedge \vec{\mathbf{d}}x^b$ results from exterior differentiation of the 1-form $\boldsymbol{\alpha} = \alpha_a \vec{\mathbf{d}}x^a$, $\vec{\mathbf{d}}\boldsymbol{\alpha} \equiv (\partial \alpha_a / \partial x^b) \vec{\mathbf{d}}x^b \wedge \vec{\mathbf{d}}x^a \Rightarrow \beta_{ab} = \partial \alpha_b / \partial x^a$. Then

$$\begin{aligned}
\mathbf{B} &\equiv \beta_{ab} \vec{dx}^a \wedge \vec{dx}^b, \quad \beta_{ab} = \partial_a \alpha_b \Rightarrow \vec{d}\mathbf{B} = \partial_c \beta_{ab} \vec{dx}^c \wedge \vec{dx}^a \wedge \vec{dx}^b, \\
&= \partial_c \partial_{[a} \alpha_{b]} \vec{dx}^c \wedge \vec{dx}^a \wedge \vec{dx}^b, \\
&= \tfrac{1}{2} (\partial_c \partial_{[a} \alpha_{b]} - \partial_a \partial_{[c} \alpha_{b]}) \vec{dx}^c \wedge \vec{dx}^a \wedge \vec{dx}^b, \\
&= \vec{d}^2 \boldsymbol{\alpha} = \mathbf{0};
\end{aligned}$$

which implies again that mixed second partial derivatives are equal: $\partial^2 \alpha_b / \partial x^c \partial x^a = \partial^2 \alpha_b / \partial x^a \partial x^c$.

In this case $\vec{d}^2 \boldsymbol{\alpha} = \mathbf{0}$ is equivalent to the vector identity $\nabla \cdot \nabla \times {}^b \mathbf{v} = \mathbf{0}$, with $\vec{d}\boldsymbol{\alpha} \equiv {}^b \mathbf{v}$:

A divergence-free vector field can be expressed as the curl of another vector field; if $\nabla \cdot {}^b \mathbf{v} = \mathbf{0}$, then ${}^b \mathbf{v}$ is *solenoidal*, or *source-free*, and a *vector potential*, say ${}^b \mathbf{p}$, can be found such that $\mathbf{v} = \nabla \times {}^b \mathbf{p}$ (Boas 1983). The statement about the vector potential is an example of the *converse of the Poincaré Lemma*: if $\boldsymbol{\gamma}$ is a p -form, $p \geq 1$, and $\vec{d}\boldsymbol{\gamma} = \mathbf{0}$, then there is a $(p-1)$ -form $\boldsymbol{\theta}$ such that $\boldsymbol{\gamma} = \vec{d}\boldsymbol{\theta}$ (Flanders 1989).

There are, however, important caveats to the Poincaré Lemma, $\vec{d}^2 \boldsymbol{\theta} = \mathbf{0}$, the first from Flanders (1989) and the second from Choquet-Bruhat, DeWitt-Morette and Dillard-Bleick (1982):

The Poincaré Lemma, $\vec{d}^2 \boldsymbol{\theta} = \mathbf{0}$, is valid in regions that are "not too complicated topologically." The lemma does not apply if the form $\boldsymbol{\theta}$ fails to be differentiable at certain points of the region.

The regions of applicability are those which are "deformable to a point" (Nash and Sen 1983, Flanders 1989). "Deformable to a point," "not too complicated topological region," and

"simply connected region" are all equivalent terms for a region \mathbf{U} of a "manifold," say \mathbf{M} , that is "star shaped." After Edelen (1977), let s^β be a set of parameters (which are just numbers)^[10] that produces *coordinates* on \mathbf{M} , say x^α (assume $\alpha = 1, \dots, n$, where n is the *dimension* of \mathbf{M}), via the n functions χ^α by the *mapping* $x^\alpha = \chi^\alpha(s^\beta)$. A region \mathbf{U} of \mathbf{M} is *star shaped* at a particular point with coordinates x_0^α if all other points x^α belonging to \mathbf{U} are such that $\zeta x^\alpha + (1 - \zeta)x_0^\alpha$ also belongs to \mathbf{U} , $0 \leq \zeta \leq 1$ is another parameter. The *radius vector*, ρ , defines the points on \mathbf{U} and can be written as $\rho \equiv x^\alpha \partial/\partial x^\alpha \equiv x^\alpha \mathbf{e}_\alpha$, where $\mathbf{e}_\alpha \equiv \partial/\partial x^\alpha$ denotes the *natural tangent basis vectors* for \mathbf{U} . So any vector can be written as $\mathbf{v} = v^\alpha \mathbf{e}_\alpha$. The *natural cotangent basis vectors* for \mathbf{U} are $\vec{d}x^\alpha$. So any 1-form ω can be written $\omega = \omega_\alpha \vec{d}x^\alpha$. Tangent $\mathbf{e}_\alpha \equiv \partial/\partial x^\alpha \equiv \vec{\partial}_\alpha$ and cotangent $\mathbf{e}^\alpha \equiv \vec{d}x^\alpha$ basis vectors for such general coordinate systems $x^\alpha = \chi^\alpha(x^a)$ will be developed for "ideal" and "defective" lattices later on.

Finally, a differential form \mathbf{B} is *closed* if its exterior derivative vanishes: $\vec{d}\mathbf{B} = \mathbf{0} \Rightarrow \mathbf{B}$ is closed. In regions of space where the Poincaré Lemma is applicable, constructing a closed form \mathbf{B} is trivial, just make it *exact* by finding some other form, say α , such that $\mathbf{B} = \vec{d}\alpha$.

A closed differential form is a higher dimensional analogue for an incompressible fluid. A closed form has no source (Arnold 1978).

[10]: Edelen (1977) uses only a single parameter s . Misner *et al.* (1973) use p parameters s^β , $\beta = 1, \dots, p$, to represent a p -dimensional region of space with say $n = 3$ dimensions; then for a surface, $p = 2$, and two parameters, s^1 and s^2 , can be used to parameterize the surface. Also, $s^\beta = s^\beta(x^a)$, since the parameters s^β can vary throughout the reference frame $\{x^a\}$.

1.3. Conservative Vector Fields

Material from the last section will be recapped with a more "standard" treatment prior to being extended.

A general covariant vector ${}^b\mathbf{v}$ (1-form) is not necessarily a "gradient," but if ${}^b\mathbf{v} = \vec{\mathbf{d}}f = (\partial f / \partial x^a)\vec{\mathbf{d}}x^a$ for some function f , then this 1-form has the property that its surfaces in one region "mesh" with those in a neighboring region, *i.e.* ${}^b\mathbf{v}$ is *conservative*. If ${}^b\mathbf{v} = \vec{\mathbf{d}}f$ then $\oint {}^b\mathbf{v} = 0$, equivalently $\vec{\mathbf{d}}{}^b\mathbf{v} = \mathbf{0}$. If, on the other hand, ${}^b\mathbf{v} = v_a \vec{\mathbf{d}}x^a$ is a Pfaffian, or *inexact* 1-form, then $\oint {}^b\mathbf{v} \neq 0$, so ${}^b\mathbf{v}$ is *non-conservative*. Differential forms, *e.g.* \mathbf{B} , are *exact* when they can be expressed as the exterior derivative of another form: \mathbf{B} is exact if $\mathbf{B} = \vec{\mathbf{d}}\alpha$ (Edelen 1985). The differential form \mathbf{B} is *closed* if $\vec{\mathbf{d}}\mathbf{B} = \mathbf{0}$. For example, if \mathbf{B} is a closed 2-form then for any closed surface \mathbf{S} in which it is defined its "tubes" are not "created" or "destroyed": $\oint_s \mathbf{B} = 0$ (Misner *et al.* 1973). The 2-form $\mathbf{B} = \beta_{ab} \vec{\mathbf{d}}x^a \wedge \vec{\mathbf{d}}x^b$ could be obtained by exterior differentiation of a 1-form $\alpha = \alpha_a \vec{\mathbf{d}}x^a$, so that $\beta_{ab} \equiv \partial \alpha_b / \partial x^a$, then $\mathbf{B} = \vec{\mathbf{d}}\alpha$, is exact, $\vec{\mathbf{d}}\mathbf{B} = \vec{\mathbf{d}}\vec{\mathbf{d}}\alpha = \mathbf{0}$, if the Poincaré Lemma holds. If, on the other hand, \mathbf{B} is inexact, then

$$\begin{aligned}\oint_s \mathbf{B} &= \text{net number of tubes of } \mathbf{B} \text{ emerging from closed surface } \mathbf{S}, \\ &= \text{number of tubes of } \mathbf{B} \text{ leaving } \mathbf{S} - \text{number of tubes of } \mathbf{B} \text{ entering } \mathbf{S}.\end{aligned}$$

For $\mathbf{B} = \beta_{ab} \vec{\mathbf{d}}x^a \wedge \vec{\mathbf{d}}x^b$ being any 2-form, the 3-form γ obtained from it by $\gamma \equiv \vec{\mathbf{d}}\mathbf{B} = (\partial \beta_{ab} / \partial x^c) \vec{\mathbf{d}}x^c \wedge \vec{\mathbf{d}}x^a \wedge \vec{\mathbf{d}}x^b$ is "tailored" to give the same number as the net number of tubes of \mathbf{B} emerging from the volume enclosed by the surface \mathbf{S} : That is, *Stokes' theorem*:

$$\int_S \mathbf{B} = \int_V \vec{d}\mathbf{B},$$

where V is the "oriented volume" which surrounds surface S . For example, if S is a surface and ∂S its boundary, then $\int_S (\nabla \times \mathbf{v}) \cdot d\mathbf{S} = \oint_{\partial S} \mathbf{v} \cdot d\mathbf{l}$ is the form of the theorem that is generally cited, $d\mathbf{S}$ and $d\mathbf{l}$ denoting "differential" surface and line "vectors," respectively.

"Defects are singularities of the field describing condensed matter. They can be identified while remaining in the regions where the field is non-singular, by generalizing the method of Stokes' and Gauss in electromagnetism, and of Burgers in elasticity theory, namely by surrounding the singularity with a closed contour (line, surface) C to obtain a non-vanishing integral of the field over C . The value of the integral is then the amount of charge, current, Burgers vector, etc. carried by the defect, and characterizes it fully, independent of the choice of C " (Rivier 1979).

A "standard" definition of the *Burgers vector*, \mathbf{b} , for a dislocation in either a continuum or crystal lattice is the line integral

$$\mathbf{b} = \oint (\partial \mathbf{u} / \partial s) ds,$$

where \mathbf{u} is the elastic displacement field, which is parameterized by s as $\mathbf{u} = \mathbf{u}(s)$ (Hirth and Lothe 1982). Evidently since $\mathbf{b} \neq 0$, \mathbf{u} is not a conservative vector field. Therefore $(\partial \mathbf{u} / \partial s) ds$

is a Pfaffian, or inexact 1-form. Thus, the indicated differentiation cannot mean an operation that one might ordinarily presume. This Pfaffian can be constructed in a variety of ways. For a dislocation in a continuum s can have any direction desired through the material. For a crystal, on the other hand, it is natural to select the parameterization to represent the crystallography.

Conservative vector fields are discussed in terms of their "integrability" for the remainder of this section, recapping results given earlier, with illustrations directed towards dislocations.

A *simply connected region* is one in which a simple closed curve can be shrunk to a point without encountering any points not in the region; it therefore has no holes (Boas 1983). For some vector field ${}^b\mathbf{v}$ with covariant components v_a such that $\partial v_a / \partial x^b$ are continuous in a simply connected region, the following five conditions are equivalent (Boas 1983):

- (1) $\nabla \times {}^b\mathbf{v} = 0$ at every point in the region;
- (2) $\oint_C {}^b\mathbf{v} \cdot d\mathbf{l} = 0$ for every simple closed curve C in the region;
- (3) \mathbf{v} is *conservative*, $\int_P^Q {}^b\mathbf{v} \cdot d\mathbf{l}$ is *independent of the path of integration*;
- (4) $\mathbf{v} \cdot d\mathbf{l}$ is an *exact differential*;
- (5) $\mathbf{v} = \nabla f$, where f is a single-valued *potential function*; $df = \nabla f \cdot d\mathbf{l} = \mathbf{v} \cdot d\mathbf{l}$
 $(v_a = \partial f / \partial x_a)$ and $\int_P^Q {}^b\mathbf{v} \cdot d\mathbf{l} = \int_P^Q df = f(Q) - f(P)$.

To use the exterior calculus (Landsberg 1990), **curl** \rightarrow **rot**, with the following considerations.

If ${}^b\mathbf{v}$ is given by exterior differentiation of some function f , ${}^b\mathbf{v} \equiv \vec{\mathbf{d}}f = (\partial f / \partial x^a) \vec{\mathbf{d}}x^a =$

$\partial_a f \vec{dx}^a$, where $v_a \equiv \partial f / \partial x^a$; then $\mathbf{0} = \vec{d}^2 f = \partial_b \partial_a f \vec{dx}^b \wedge \vec{dx}^a = \frac{1}{2} (\partial_b \partial_a f - \partial_a \partial_b f) \vec{dx}^b \wedge \vec{dx}^a$

is equivalent to $\text{rot } \mathbf{v} = \mathbf{0}$:

$$\begin{aligned}
\text{rot } \mathbf{v} &\equiv \vec{d}^b \mathbf{v} = \vec{d}(v_a \vec{dx}^a), \\
&= \vec{d} v_a \wedge \vec{dx}^a, \\
&= (\partial v_a / \partial x^b) \vec{dx}^b \wedge \vec{dx}^a, \\
&= \frac{1}{2} (\partial v_a / \partial x^b - \partial v_b / \partial x^a) \vec{dx}^b \wedge \vec{dx}^a, \\
&\equiv \partial_{[b} v_{a]} \vec{dx}^b \wedge \vec{dx}^a, \\
(\partial_{[b} v_{a]} &\equiv \frac{1}{2} [\partial v_a / \partial x^b - \partial v_b / \partial x^a] \equiv \frac{1}{2} [\partial_b v_a - \partial_a v_b]) \\
&\equiv v_{[a,b]} \vec{dx}^b \wedge \vec{dx}^a, \\
(v_{[a,b]} &\equiv \frac{1}{2} [v_{a,b} - v_{b,a}] \equiv \frac{1}{2} [\partial v_a / \partial x^b - \partial v_b / \partial x^a]) \\
&= (v_{z,y} - v_{y,z}) \vec{dy} \wedge \vec{dz} + (v_{x,z} - v_{z,x}) \vec{dz} \wedge \vec{dx} + (v_{y,x} - v_{x,y}) \vec{dx} \wedge \vec{dy};
\end{aligned}$$

then $\partial v_a / \partial x^b - \partial v_b / \partial x^a = \partial(\partial_a f) / \partial x^b - \partial(\partial_b f) / \partial x^a = 0$. When \mathbf{b}_v is exact, $\mathbf{b}_v \equiv \vec{d}f = (\partial f / \partial x^a) \vec{dx}^a$, and the integral $\int_P^Q \mathbf{b}_v \equiv \int_P^Q df = f(Q) - f(P)$ is path independent; \mathbf{b}_v is then called *curl-free*, not "rotation-free" (Misner *et al.* 1973). The condition $\text{rot } \mathbf{v} = \vec{d}^b \mathbf{v} = \vec{d}^2 f = \mathbf{0}$, is equivalent to $\nabla \times \mathbf{b}_v = \nabla \times \mathbf{b}_f = \mathbf{0}$, which is the Poincaré Lemma again.

This condition of curl-free ($\vec{d}^b \mathbf{v} = \mathbf{0}$) vector \mathbf{b}_v giving the existence of a function f such that $\mathbf{b}_v = \vec{d}f$ is only *necessary* for exactness, it is not *sufficient*. For example, suppose that in two dimensions $\vec{d}^b \mathbf{v} = \mathbf{0}$ ($\nabla \times \mathbf{b}_v = \mathbf{0}$) in some "region" with a hole in it. Then $\mathbf{b}_v = \vec{d}f$ ($\mathbf{b}_v = \mathbf{b}_f$) cannot generally be satisfied by a single function f because of the hole: the line integral $\oint \mathbf{b}_v$ will not generally vanish (Edelen 1985). This is the problem of a

dislocation in either a crystal or an elastic continuum: *e.g.* an edge dislocation is an extra half-plane.

A dislocation can only be made in a continuum if the body is multiply-connected: *i.e.* if there is a tube of material cut out of the body around the dislocation core (Nabarro 1967). **Crystalline line defects can be modelled as strain singularities in an elastic continuum** (Kröner and Anthony 1975).

A p -form α is closed if $\vec{d}\alpha = 0$. It is exact if there exists a $(p - 1)$ -form \mathbf{B} such that $\alpha = \vec{d}\mathbf{B}$ (Edelen 1985). All differential forms are integrands, but only exact forms are independent of the integration path. A curl-free 1-form is exact, or the "gradient" of some function. A *rotation-free* 1-form (this is some bad terminology— ${}^b\mathbf{v}$ is rotation-free does not mean $\text{rot } \mathbf{v} = \mathbf{0}$) is not necessarily exact, *i.e.* it may not be a gradient of any function; but it can be made into a gradient by multiplying it by some function, say I , called an *integrating factor*. Suppose then that ${}^b\mathbf{v} \equiv v_a \vec{d}x^a$ is not exact, but that $I {}^b\mathbf{v} \equiv {}^b\mathbf{w} \equiv w_a \vec{d}x^a$ is. Then ${}^b\mathbf{w}$ is a "gradient" of some function, say g , ${}^b\mathbf{w} \equiv \vec{d}g = (\partial g / \partial x^a) \vec{d}x^a \Rightarrow I v_a = \partial g / \partial x^a \Rightarrow {}^b\mathbf{v} = I^{-1} \vec{d}g$. Thus, $\int_P^Q I {}^b\mathbf{v} = \int_P^Q \vec{d}g = g(Q) - g(P)$. Therefore, ${}^b\mathbf{v} = I^{-1} \vec{d}g \Rightarrow \vec{d}{}^b\mathbf{v} = \vec{d}I^{-1} \wedge \vec{d}g$, and since $\omega \wedge \omega = \mathbf{0}$ (the wedge product is antisymmetric),

$${}^b\mathbf{v} \wedge \vec{d}{}^b\mathbf{v} = \mathbf{0}.$$

This expression has the components

$$v_{[a,b]}v_c + v_{[b,c]}v_a + v_{[c,a]}v_b = 0,$$

or "standard" vector representation^[11]

$$\mathbf{v} \cdot \nabla \times {}^b\mathbf{v} = \mathbf{0}.$$

The expressions $\mathbf{v} \cdot \nabla \times {}^b\mathbf{v} = \mathbf{0}$ and ${}^b\mathbf{v} \wedge \vec{\mathbf{d}} {}^b\mathbf{v} = \mathbf{0}$ are equivalent statements of the *Frobenius theorem* (Misner *et al.* 1973), which is the topic of the next subsection.

The Frobenius theorem is concerned with the "integrability" of a system of partial differential equations (Levi-Cevita 1977): If $\mathbf{v} \cdot \nabla \times {}^b\mathbf{v} = \mathbf{0}$ then ${}^b\mathbf{v} = v_a \vec{\mathbf{d}} x^a = \mathbf{0}$ is equivalent to $\vec{\mathbf{d}} g = \partial_a g \vec{\mathbf{d}} x^a = \mathbf{0}$, where ${}^b\mathbf{v} = I^{-1} \vec{\mathbf{d}} g$, and $g(x^a) = \text{constant}$ is the *integral* of the Pfaffian ${}^b\mathbf{v} = \mathbf{0}$. The relationship $g(x^a) = \text{constant}$ defines a plane: if $g(x^a)$ is some point ρ , so $\rho = g(x^a)$, and $\rho + \Delta\rho = g(x^a + \Delta x^a)$ is a neighboring point on this plane, then $g(x^a) = g(x^a + \Delta x^a) = \text{constant}$ implies that $(\partial g / \partial x^a) \Delta x^a = 0$, or $\vec{\mathbf{d}} g = (\partial g / \partial x^a) \vec{\mathbf{d}} x^a = \mathbf{0}$. Bilby *et al.* (1958) present some applications of the Frobenius theorem to dislocation theory.

[11]: Since $Iv_a = \partial_a g$,

$$\vec{\mathbf{d}}^2 g = \frac{1}{2}(\partial_b \partial_a g - \partial_a \partial_b g) \vec{\mathbf{d}} x^b \wedge \vec{\mathbf{d}} x^a = \mathbf{0}$$

gives

$$\begin{aligned} \mathbf{0} &= \vec{\mathbf{d}}^2 g = \frac{1}{2}[\partial_b(Iv_a) - \partial_a(Iv_b)] \vec{\mathbf{d}} x^b \wedge \vec{\mathbf{d}} x^a, \\ &= \frac{1}{2}[(\partial_b I)v_a + I\partial_b v_a - (\partial_a I)v_b - I\partial_a v_b] \vec{\mathbf{d}} x^b \wedge \vec{\mathbf{d}} x^a, \end{aligned}$$

which implies that $I(\partial_b v_a - \partial_a v_b) = v_b(\partial_a I) - v_a(\partial_b I)$, or, multiplying by v_c ,

$v_c I(\partial_b v_a - \partial_a v_b) = v_c[v_b(\partial_a I) - v_a(\partial_b I)]$. Interchanging the indices a,b,c, and adding up the three terms results in (Landsberg 1990)

$$v_c I(\partial_b v_a - \partial_a v_b) + v_b I(\partial_a v_c - \partial_c v_a) + v_a I(\partial_c v_b - \partial_b v_c) = 0 \Rightarrow \mathbf{v} \cdot \nabla \times {}^b\mathbf{v} = \mathbf{0}.$$

Simple "Integrability Conditions"

A simple illustration of "integrability conditions" follows from considering a crystallographic coordinate system, $X^M = X, Y, Z$, for conventional unit cells in a cubic crystal. Tangent basis vectors $\mathbf{A}_M \equiv A_M \mathbf{I}_M$ (no sum) define the unit cell which is a simple cube, the $A_M = A_x = A_y = A_z \equiv A$ are the lattice parameters and the \mathbf{I}_M are the associated unit vectors. Cotangent basis vectors are the "gradients" $\mathbf{A}^M \equiv A^M \mathbf{I}^M \equiv \vec{\mathbf{d}}X^M \equiv {}^b\nabla X^M = (\partial X^M / \partial x^a) \mathbf{i}^a$. The relationships $A_M = A = 1/A^M$ and $\mathbf{I}_M = \mathbf{I}^M$ hold because the X^M coordinates are orthogonal. Tangent and cotangent basis vectors can therefore be related as $\mathbf{A}_L = \mathbf{A}_M \times \mathbf{A}_N$ and $\mathbf{A}^L = \mathbf{A}^M \times \mathbf{A}^N$, respectively, for even permutations (123, 231, 312) of L,M,N. The curl $\nabla \times$ of any gradient is identically zero;

$$\nabla \times {}^b\nabla X^M = \nabla \times \mathbf{A}^M = \mathbf{0}$$

is an "integrability condition." Another vector identity is $\nabla \cdot ({}^b\nabla f \times {}^b\nabla g) = 0$, for any functions f and g ; so

$$\nabla \cdot ({}^b\nabla X^M \times {}^b\nabla X^N) = \nabla \cdot {}^b\nabla X^L = \nabla \cdot \mathbf{A}^L = 0$$

is another "integrability condition." The X^M coordinates are curl-free, divergence-free, "conserved," and *holonomic*.

1.4. The Frobenius Theorem

Compatibility conditions are first order integrability conditions.

The Frobenius theorem is used to answer the question of existence and uniqueness of *overdetermined systems of partial differential equations* (Abraham, Marsden, and Ratiu 1988). For example, consider p functions

$$\chi^\alpha = \chi^\alpha(x, y, z), \alpha = 1, 2, \dots, p,$$

that are to be determined by solving the differential equations

$$d\chi^\alpha / dx^a \equiv \lambda_a^\alpha(x, y, z; \chi^1, \chi^2, \dots, \chi^p).$$

Is there in fact a solution $\chi^\alpha = \chi^\alpha(x^a; c^\alpha)$ for any choice of initial conditions, c^α , such that $\chi^\alpha(\dots, \dots, \dots; c^\alpha) = c^\alpha$? This system of differential equations just says that $\vec{d}\chi^\alpha = \lambda_a^\alpha \vec{d}x^a$; it is therefore equivalent to the *Pfaffian system*

$$\vec{d}\chi^\alpha = \lambda_a^\alpha \vec{d}x^a \Rightarrow \gamma^\alpha \equiv \vec{d}\chi^\alpha - \lambda_a^\alpha \vec{d}x^a \equiv 0, \lambda_a^\alpha = \partial \chi^\alpha / \partial x^a.$$

Here, each of the p objects $\gamma^\alpha = (\mathbf{0}^1, \mathbf{0}^2, \dots, \mathbf{0}^p)$ is a 1-form, the index α indicates which 1-form, and not any particular components. For such a Pfaffian system the Frobenius theorem takes the form of

$$\vec{d}\gamma^\alpha \wedge \gamma^1 \wedge \dots \wedge \gamma^p = 0, \alpha = 1, \dots, p,$$

which if true, indicates the existence of a $p \times p$ matrix of 1-forms $\Gamma_{ba}^\alpha \vec{d}x^a$,

$$\Gamma_{ba}^\alpha \vec{d}x^a = \begin{vmatrix} \Gamma_{1a}^1 \vec{d}x^a & \Gamma_{1a}^2 \vec{d}x^a & \dots & \Gamma_{1a}^p \vec{d}x^a \\ \Gamma_{2a}^1 \vec{d}x^a & \Gamma_{2a}^2 \vec{d}x^a & \dots & \Gamma_{2a}^p \vec{d}x^a \\ \Gamma_{3a}^1 \vec{d}x^a & \Gamma_{3a}^2 \vec{d}x^a & \dots & \Gamma_{3a}^p \vec{d}x^a \\ \dots & \dots & \dots & \dots \\ \Gamma_{pa}^1 \vec{d}x^a & \Gamma_{pa}^2 \vec{d}x^a & \dots & \Gamma_{pa}^p \vec{d}x^a \end{vmatrix},$$

such that

$$\vec{d}\gamma^\alpha = \Gamma_{ba}^\alpha \vec{d}x^a \wedge \gamma^b,$$

and the system of equations $\gamma^\alpha = 0$ is therefore *completely integrable* (Edelen 1977). Taking the exterior derivative of $\gamma^\alpha = \vec{d}\chi^\alpha - \lambda^a \vec{d}x^a$ yields (Abraham *et al.* 1988)

$$\vec{d}\gamma^\alpha = \frac{1}{2} Y_{ab}^\alpha \vec{d}x^a \wedge \vec{d}x^b + \Gamma_{ba}^\alpha \vec{d}x^a \wedge \gamma^b,$$

where

$$\begin{aligned} Y_{ab}^\alpha &\equiv \partial_b \lambda_a^\alpha - \partial_a \lambda_b^\alpha + (\partial_b \lambda_a^\alpha) \lambda_b^\beta - (\partial_b \lambda_b^\alpha) \lambda_a^\beta, \\ &\equiv T_{ba}^\alpha + (\Gamma_{ba}^\alpha \lambda_b^\beta - \Gamma_{bb}^\alpha \lambda_a^\beta), \end{aligned}$$

with $\partial_\beta \equiv \partial/\partial\chi^\beta$, and

$$\Gamma_{ba}^\alpha \equiv \partial_b \lambda_a^\alpha \text{ and, } T_{ba}^\alpha \equiv \partial_b \lambda_a^\alpha - \partial_a \lambda_b^\alpha.$$

The Frobenius theorem is consequently satisfied if $\Upsilon_{ab}^\alpha = 0$, since $\vec{d}\Upsilon^\alpha = \Gamma_{\beta a}^\alpha \vec{d}x^a \wedge \Upsilon^\beta$ implies that $\vec{d}\Upsilon^\alpha \wedge \Upsilon^\beta = 0$, $\Upsilon^\beta \wedge \Upsilon^\beta$ vanishing because the wedge product is antisymmetric. The equations $\Upsilon_{ab}^\alpha = 0$ are *compatibility conditions* for the system of equations $\Upsilon^\alpha = \vec{d}\chi^\alpha - \lambda_a^\alpha \vec{d}x^a = 0$; they are *first order integrability conditions* (Bryant *et al.* 1991).

The system of equations [$\Upsilon^\alpha = \vec{d}\chi^\alpha - \lambda_a^\alpha \vec{d}x^a = 0$] will not always be completely integrable.